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Study of the environment of Fe3+ in Na2Cd(SO 4)2 2H2O by EPR

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Abstract

An EPR experiment on Fe3+ in a single crystal of Na 2Cd(SO4)2 2H2O was carried out at Q band frequency and nitrogen temperature. The angular dependencies of the spectra were studied in the three crystallographic planes. In order to have a very precise orientation of the crystal, the experiment was done with a twinned crystal (superposition of two spectra in all three planes). The zero-field splitting of Fe3+ is of the same order of magnitude as the quantum hv, so that many ΔM=2 transitions were observed. All spin-Hamiltonian parameters (20) were calculated using observed ΔM=1 and ΔM=2 transitions for 30 different orientations of the magnetic field. The pseudosymmetries of the fourth-order term of the spin Hamiltonian of Fe 3+ are compared to those we calculated using the superposition model. It is seen that Fe3+ is substituted for Cd2+ and that the orientation of the ocatahedral environment of Fe3+ does not differ much in orientation from that of Cd2+. Differences between the distortions of the Cd-O6 and Fe-O6 octahedra are discussed.